3-CF3-C6H4-COOCH3

Other names: 3-CF3-C6H4-COOCH3
Inchi: InChI=1S/C9H7F3O2/c1-14-8(13)6-2-4-7(5-3-6)9(10,11)12/h2-5H,1H3
InchiKey: VAZWXPJOOFSNLB-UHFFFAOYSA-N
Formula: C9H7F3O2
SMILES: COC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 204.15

Physical Properties

Property code	Value	Unit	Source
af	0.4852		Cheméo Relay (1.0)
affp	827.50	kJ/mol	NIST Webbook
basg	796.50	kJ/mol	NIST Webbook
ea	0.75 ± 0.09	eV	NIST Webbook
ea	0.72 ± 0.09	eV	NIST Webbook
hf	-937.02	kJ/mol	Cheméo Relay (1.0)
hfus	17.33	kJ/mol	Joback Method
hvap	62.37	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
log10ws	-2.93		Cheméo Relay (1.0)
logp	2.492		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	471.37	K	Cheméo Relay (1.0)
tc	663.41	K	Cheméo Relay (1.0)
tf	333.12	K	Cheméo Relay (1.0)
vc	0.462	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.63	J/mol×K	507.85	Joback Method
cpg	295.99	J/mol×K	540.87	Joback Method
cpg	306.64	J/mol×K	573.90	Joback Method
cpg	316.61	J/mol×K	606.92	Joback Method

cpg	325.92	J/mol×K	639.95	Joback Method
cpg	334.60	J/mol×K	672.97	Joback Method
cpg	342.69	J/mol×K	706.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2967660&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume